L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
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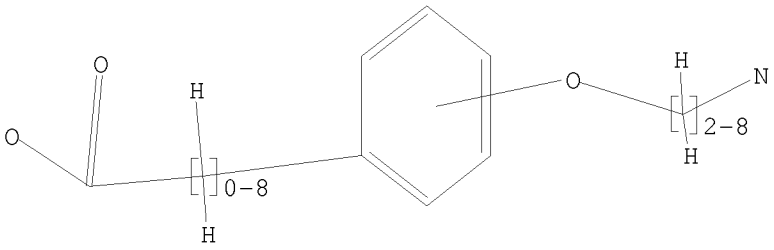


Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 13:55:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2635465 TO ITERATE

35.9% PROCESSED 945815 ITERATIONS 975 ANSWERS

37.9% PROCESSED 1000000 ITERATIONS 1017 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.22

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 2635465 TO 2635465
PROJECTED ANSWERS: 2525 TO 2835

L2 1017 SEA SSS FUL L1

L3 116 L2

=> s l3 and py<2002
21992686 PY<2002
L4 6 L3 AND PY<2002

=> s l1 full
REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 13:56:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2635465 TO ITERATE

36.4% PROCESSED 959447 ITERATIONS 975 ANSWERS

37.9% PROCESSED 1000000 ITERATIONS 1017 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.22

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 2635465 TO 2635465
PROJECTED ANSWERS: 2525 TO 2835

L5 1017 SEA SSS FUL L1

L6 116 L5

=> s l3 and py<2002
21992686 PY<2002
L7 6 L3 AND PY<2002

=> d 1-6 ibib abs hitstr

L7 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2008:208799 CAPLUS
DOCUMENT NUMBER: 148:275678
TITLE: Vitronectin receptor antagonist pharmaceuticals
INVENTOR(S): Rajopadhye, Milind; Barrett, John A.; Carpenter, Jr., Alan P.; Cheesman, Edward H.; Harris, Thomas D.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Pharma Company, USA
SOURCE: U.S., 133pp., Cont.-in-part of U.S. Ser. No. 466,588.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
US 7332149	B1	20080219	US 2000-599890	20000621	
US 6322770	B1	20011127	US 1999-281207	19990330	<--
US 20020015680	A1	20020207	US 1999-281209	19990330	
US 6524553	B2	20030225			
US 6548663	B1	20030415	US 1999-281050	19990330	
US 6794518	B1	20040921	US 1999-466588	19991217	
US 20030124120	A1	20030703	US 2002-269252	20021011	

US 20030149262	A1	20030807	US 2002-306054		20021126
US 20050154185	A1	20050714	US 2004-770380		20040202
US 7321045	B2	20080122			
PRIORITY APPLN. INFO.:			US 1998-112829P	P	19981218
			US 1999-466588	A2	19991217
			US 1998-80150P	P	19980331
			US 1998-112715P	P	19981218
			US 1998-112732P	P	19981218
			US 1998-112831P	P	19981218
			US 1999-281050	A3	19990330
			US 1999-281209	A3	19990330

GI

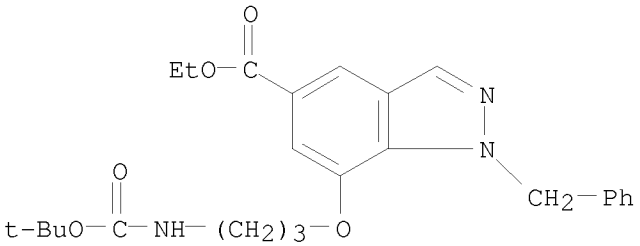
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention describes novel compds. comprising at least one of a chemotherapeutic agent or a radiosensitizer agent, and further comprising a diagnostic or therapeutic metallopharmaceutical selected from defined 99mTc complexes, e.g., 99mTc(L)(tricine)(TPPTS) where L = diazenido derivative of polyfunctional benzenesulfonic acid I and TPPTS = tris(m-sulfophenyl)phosphine trisodium salt, or various indium, lutetium, yttrium or gadolinium polyfunctionalized DOTA-type complexes, e.g., indium complex II, useful for the diagnosis and treatment of cancer, methods of imaging tumors in a patient, and methods of treating cancer in a patient. The pharmaceuticals are thus comprised of a targeting moiety that binds to the vitronectin receptor that is expressed in tumor vasculature, an optional linking group, and a therapeutically effective radioisotope or diagnostically effective imageable moiety. The present invention also provides novel compds. useful for monitoring therapeutic angiogenesis treatment and destruction of new angiogenic vasculature. The present invention also provides novel compds. useful for imaging atherosclerosis, restenosis, cardiac ischemia, and myocardial reperfusion injury. The present invention also provides novel compds. useful for the treatment of rheumatoid arthritis. The pharmaceuticals are comprised of a targeting moiety that binds to a receptor that is upregulated during angiogenesis, an optional linking group, and a therapeutically effective radioisotope or diagnostically effective imageable moiety. The imageable moiety is a gamma ray or positron emitting radioisotope, a magnetic resonance imaging contrast agent, an x-ray contrast agent, or an ultrasound contrast agent.

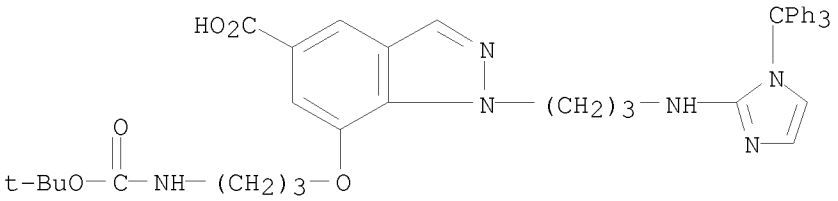
IT 1007219-80-8P 1007219-81-9P
RL: PRPH (Prophetic); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(vitronectin receptor antagonist metallopharmaceuticals as chemotherapeutic or radiosensitizer agents)

RN 1007219-80-8 CAPLUS

CN 1H-Indazole-5-carboxylic acid, 7-[3-[[(1,1-dimethylethoxy)carbonyl]amino]propoxy]-1-(phenylmethyl)-, ethyl ester (CA INDEX NAME)



RN 1007219-81-9 CAPLUS
CN 1H-Indazole-5-carboxylic acid, 7-[3-[[(1,1-dimethylethoxy)carbonyl]amino]propoxy]-1-[3-[[1-(triphenylmethyl)-1H-imidazol-2-yl]amino]propyl]- (CA INDEX NAME)



REFERENCE COUNT: 148 THERE ARE 148 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:12266 CAPLUS
DOCUMENT NUMBER: 134:86149
TITLE: Preparation of diphenyl ureas as VLA-4 inhibitors
INVENTOR(S): Baldwin, John J.; McDonald, Edward; Moriarty, Kevin Joseph; Sarko, Christopher Ronald; Machinaga, Nobuo; Nakayama, Atsushi; Chiba, Jun; Iimura, Shin; Yoneda, Yoshiyuki
PATENT ASSIGNEE(S): Daiichi Pharmaceutical Co., Ltd., Japan; Pharmacopeia, Inc.
SOURCE: PCT Int. Appl., 511 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001000206	A1	20010104	WO 2000-US18079	20000630 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2369308	A1	20010104	CA 2000-2369308		20000630 <--
EP 1189612	A1	20020327	EP 2000-945035		20000630
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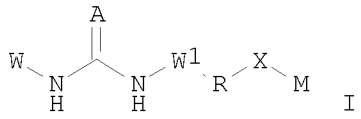
BR 2000012068	A	20020514	BR 2000-12068		20000630
JP 2003503350	T	20030128	JP 2001-505915		20000630
AU 781438	B2	20050526	AU 2000-59031		20000630
RU 2264386	C2	20051120	RU 2001-135856		20000630
TW 283240	B	20070701	TW 2000-89112968		20000630
IL 146288	A	20080210	IL 2000-146288		20000630
ZA 2001009203	A	20030207	ZA 2001-9203		20011107
MX 2001013406	A	20030904	MX 2001-13406		20011219
NO 2001006319	A	20020228	NO 2001-6319		20011221
NO 324892	B1	20071227			
US 20030078249	A1	20030424	US 2001-34585		20011228
US 6756378	B2	20040629			
US 20040229858	A1	20041118	US 2004-787905		20040226
US 7179819	B2	20070220			
US 20070054909	A1	20070308	US 2006-594432		20061108
PRIORITY APPLN. INFO.:			US 1999-141601P	P	19990630
			US 1999-141602P	P	19990630
			US 1999-141692P	P	19990630
			WO 2000-US18079	W	20000630
			US 2001-34585	A3	20011228
			US 2004-787905	A3	20040226

OTHER SOURCE(S): MARPAT 134:86149

GI



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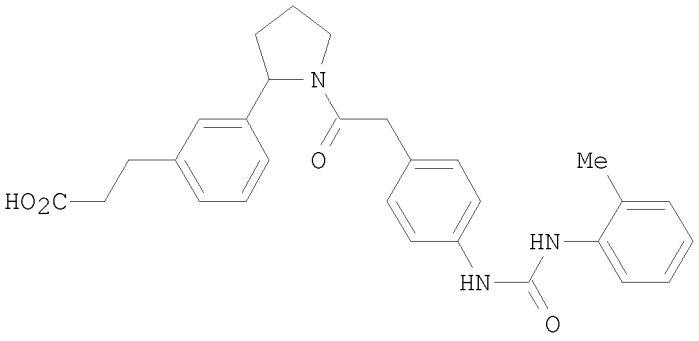


II

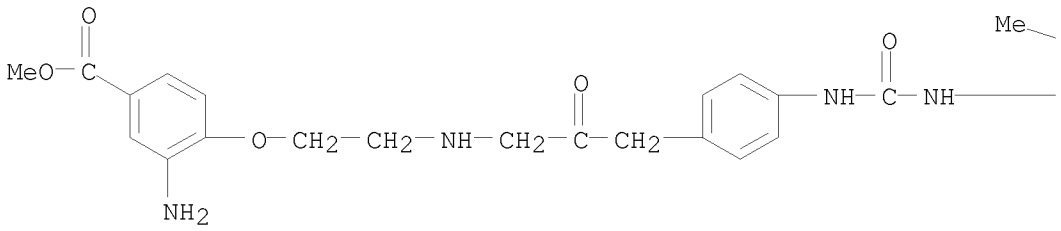
AB The title compds. [I; W = (un)substituted aryl, heteroaryl; W1 = (un)substituted arylene, heteroarylene; A = O, S, NH; R = a bond, alkenylene, (CH2)n; n = 1-2; X = CO, CH2, SO2; M = substituted pyrrolidinyl, thiazolidinyl, etc.] which selectively inhibit the binding of ligands to α4β1 integrin (VLA-4), and therefore are useful in the treatment of conditions associated with VLA-4 mediated cell adhesion, including, but not limited to, such conditions as inflammatory and autoimmune responses, diabetes, asthma, psoriasis, inflammatory bowel disease, transplantation rejection, and tumor metastasis, were prepared E.g., a multi-step synthesis of the urea II which showed Ki of < 50 nM against VLA-4 receptors binding, was given.

IT 1101107-01-0
RL: PRPH (Prophetic)
(Preparation of diphenyl ureas as VLA-4 inhibitors)

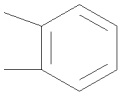
RN 1101107-01-0 CAPLUS

CN Benzoic acid, 3-amino-4-[2-[[3-[4-[[[(2-methylphenyl)amino]carbonyl]amino]phenyl]-2-oxopropyl]amino]ethoxy]-, methyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1998:682372 CAPLUS
DOCUMENT NUMBER: 129:316232
ORIGINAL REFERENCE NO.: 129:64535a,64538a
TITLE: Preparation of compounds and compositions for treating diseases associated with serine protease, particularly tryptase, activity
INVENTOR(S): Church, Timothy J.; Cutshall, Neil Scott; Gangloff, Anthony R.; Jenkins, Thomas E.; Linsell, Martin S.; Litvak, Joane; Rice, Kenneth D.; Spencer, Jeffrey R.; Wang, Vivian R.
PATENT ASSIGNEE(S): Axys Pharmaceuticals Corporation, USA

SOURCE: PCT Int. Appl., 108 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9845275	A1	19981015	WO 1997-US21849	19971201 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2285454	A1	19981015	CA 1997-2285454	19971201 <--
AU 9858950	A	19981030	AU 1998-58950	19971201 <--
AU 752064	B2	20020905		
CN 1251579	A	20000426	CN 1997-182098	19971201 <--
EE 9900477	A	20000615	EE 1999-477	19971201 <--
EE 4055	B1	20030616		
EP 1019382	A1	20000719	EP 1997-954520	19971201 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
NZ 500029	A	20010223	NZ 1997-500029	19971201 <--
HU 2000001522	A2	20010528	HU 2000-1522	19971201 <--
HU 2000001522	A3	20010828		
JP 2001519806	T	20011023	JP 1998-542739	19971201 <--
MX 9909006	A	20000831	MX 1999-9006	19991001 <--
NO 9904858	A	19991206	NO 1999-4858	19991006 <--
NO 314183	B1	20030210		
LV 12495	B	20010120	LV 1999-153	19991102 <--
LT 4704	B	20000925	LT 1999-131	19991105 <--
US 20010053779	A1	20011220	US 2001-874412	20010604 <--
US 6562854	B2	20030513		
US 20030212120	A1	20031113	US 2003-401415	20030314

PRIORITY APPLN. INFO.:

US 1997-833674	A	19970407
US 1994-357491	B2	19941214
US 1997-980515	A1	19971201
WO 1997-US21849	W	19971201
US 2001-874412	A1	20010604

OTHER SOURCE(S): CASREACT 129:316232; MARPAT 129:316232

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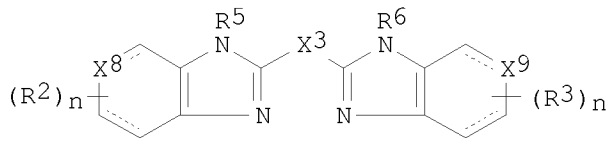


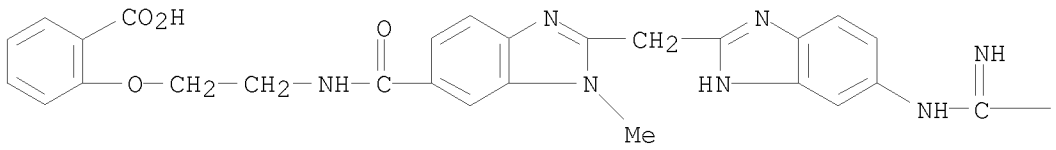
I

AB A preferred aspect of the invention are compds. of Formula [I; in which: the dashed lines independently represent optional bonds; each R2 independently is (C1-6)alkyl, (C1-6)alkyloxy, halo or hydroxy; each R3 independently is (C1-6)alkyl, (C1-6)alkyloxy, halo or hydroxy; X3 is -C(O)- or -CR7R8-, X8 is -CH(R1)n1- or -C(R1)n1=, wherein R1 is amino(N1-4)azolidinyl, amino(N1-4)azolyl, (N1-4)azolidinyl, (N1-4)azolyl, etc.; X8 is -N= or -NH(R1)n1-, wherein R1 is -C(NR9)R9, -C(NH)NHR10 or -C(NH)NR10R10, wherein R9 independently is hydrogen or (C1-6)alkyl and each R10 independently is (C1-6)alkyl; and X9 is -CH(R4)- or -C(R4)=, wherein R4 is -R12, -OR12, -N(R13)R12, etc.; wherein R4 is -C(O)R12, -C(O)OR12, -C(O)N(R13)R12, etc.; R12 is cyano, guanidino, halo, alkyl, etc.; R13 is hydrogen, alkyl; R5 is hydrogen or (C1-4)alkyl, R6 is hydrogen or (C1-4) alkyl; R7 is hydrogen, methyl; R8 is hydrogen Me, hydroxy; n = 0-4]. The compds., compns. and methods are effective for the prevention and treatment of inflammatory diseases associated with the respiratory tract, such as asthma and allergic rhinitis, as well as other types of immunomediated inflammatory disorders, such as rheumatoid arthritis, conjunctivitis and inflammatory bowel disease, various dermatol. conditions, as well as certain viral conditions. The compds. comprise potent and selective inhibitors of the mast-cell protease tryptase. The compns. for treating these conditions include oral, inhalant, topical and parenteral prepns. as well as devices comprising such prepns.

IT 1101453-56-8 1101453-66-0
RL: PRPH (Prophetic)
(Preparation of compounds and compositions for treating diseases associated with serine protease, particularly tryptase, activity)

RN 1101453-56-8 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

PAGE 1-A



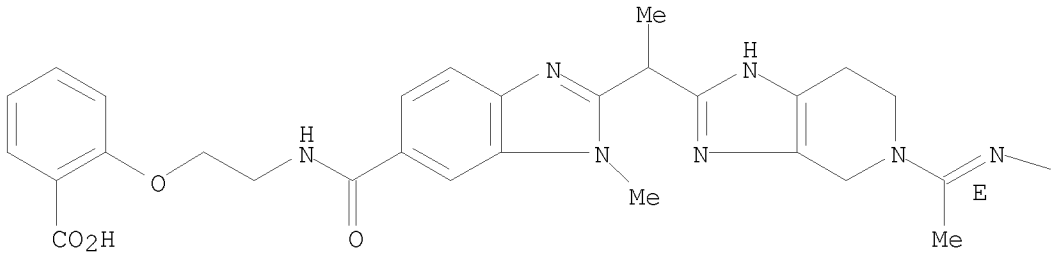
PAGE 1-B

— NH_2

RN 1101453-66-0 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B

OH

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1966:20052 CAPLUS
DOCUMENT NUMBER: 64:20052
ORIGINAL REFERENCE NO.: 64:3741b-g
TITLE: Aminoarylideneacetonitrile dyes
PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.
SOURCE: 16 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6500517		19650719	NL 1965-517	19650115 <--
BE 658426			BE	
FR 1425609			FR	
PRIORITY APPLN. INFO.:			DE	19640117

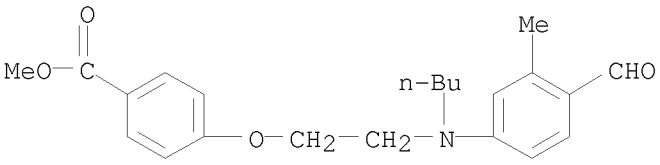
GI For diagram(s), see printed CA Issue.
AB Greenish yellow dyes of the general formula I for polyester fabrics were prepared; in formula I, R is H or Me, R1 Et, Bu, or PhOCH2CH2, R2 = H or MeO2C, X = CN or CO2Et, and Y is CO2, OCO2, or O. Bu(HOCH2CH2)NPh (II) 19.3, C6H6 100, powdered K2CO3 13.8, present with p-MeO2CC6H4COCl 19.9 parts, and the product 35.5 parts, b0.6 230-5°, in 100 parts PhCl added dropwise at 50-5° to 30.7 parts POCl3 and 14.6 parts HCONMe2 and stirred 12 hrs. at 50-5° yielded p-MeO2CC6H4CO2CH2CH2N(Br)C6H4CHO-p (III). III 38, NCCH2CO2Et 12, EtOH 20, and piperidine 1 part refluxed 2 hrs. yielded yellow I (R = H, R1 = Bu, R2 = p-MeO2C, X = CO2Et, Y = CO2), m. 120-1° (EtOH); it dyes polyester, polyamide, and triacetylcellulose fabrics greenish yellow shades of very good fastness

properties. III with CH2(CN)2 gave similarly I (R = H, R1 = Bu, R2 = p-MeO2C, X = CN, Y = CO2), m. 88-90°. II (20.7 parts) treated with 19.9 parts p-MeO2CC6H4COCl and 11 parts Et3N at 80-100°, and the condensation product formylated yielded 2,4-Me[p-MeO2CC6H4CO2CH2CH2N(Bu)]C6H3CHO; a 40-part portion in 100 cc. Et3N with 7 parts CH2(CN)2 in BuOH yielded greenish yellow I (R = Me, R1 = Bu, R2 = MeO2C, X = CN, Y = CO2), m. 112-14° (EtOH). Et(HOCH2CH2)NPh condensed with o-MeO2CC6H4COCl and then formylated, and the resulting 2,4-Me[o-MeO2CC6H4CO2CH2CH2N(Et)]C6H3CHO treated with CH2(CN)2 yielded I (R = Me, R1 = Et, R2 = o-MeO2C, X = CN, Y = CO2), m. 100-1°. 3-Me derivative of II condensed with p-ClCO2C6H4CO2Me, and the product heated to 150-200°, distilled (b0.5-0.6 198-207°), and then formylated with POCl3-HCONMe2 gave 2,4-Me[p-MeO2CC6H4OCH2CH2N(Bu)]C6H3CHO, b1.6 279-80°, which with CH2(CN)2 yielded I (R = Me, R1 = Bu, R2 = p-MeO2C, X = CN, Y = O), m. 84-7°. m-MeC6H4N(CH2CH2Cl)Et (IV) 59.5, HCONMe2 100, and PhONa 34.8 parts gave m-McC6H4N(CH2CH2OPh)Et, b0.8 155-63°, which formylated and condensed with NCCH2CO2Et yielded I (R = Me, R1 = Et, R2 = H, X = CO2Et, Y = O), m. 74-5°. IV 59.8, HCONMe2 357, and p-MeO2CC6H4CO2K 72.5 parts heated 7 hrs. at 140°, concentrated, and treated with 95 parts POCl3 yielded 2,4-Me[p-MeO2CC6H4CO2CH2CH2N(Et)]C6H3CHO, m. 77-80°, which condensed with CH2(CN)2 yielded I (R = Me, R1 = Et, R2 = p-EtO2C, X = CN, Y = CO2), m. 136-8°. m-MeC6H2N(CH2CH2OH)Et 71.5 with ClCO2Ph 69.0 and Et3N 44.5 parts gave m-MeC6H3N(CH2CH2OCO2Ph)Et which formylated and condensed with CH2(CN)2 yielded I (R = Me, R1 = Et, R2 = H, X = CN, Y = OCO2). m-MeC6H4(CH2CH2Cl)2 23.2, NaOPh 24, and (MeOCH2CH2)2O 50 parts refluxed 1-2 hrs., and the product formylated gave 2,4-Me[(PhOCH2CH2)2N]C6H3CHO, m. 82-4° (EtOH), which condensed with CH2(CN)2 yielded I (R = Me, R1 = PhOCH2CH2, R2 = H, X = CN, Y = O); it dyes greenish yellow shades.

IT 1081794-87-7P
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(Aminoarylideneacetonitrile dyes)

RN 1081794-87-7 CAPLUS

CN Benzoic acid, 4-[2-[butyl(4-formyl-3-methylphenyl)amino]ethoxy]-, methyl ester (CA INDEX NAME)



L7 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1959:6864 CAPLUS
DOCUMENT NUMBER: 53:6864
ORIGINAL REFERENCE NO.: 53:1257c-i
TITLE: Lower-alkyl 5-amino-2-(tertiary aminoalkoxy)benzoates
INVENTOR(S): Clinton, Raymond O.; Laskowski, Stanley C.
PATENT ASSIGNEE(S): Sterling Drug Inc.
DOCUMENT TYPE: Patent

LANGUAGE: Unavailable
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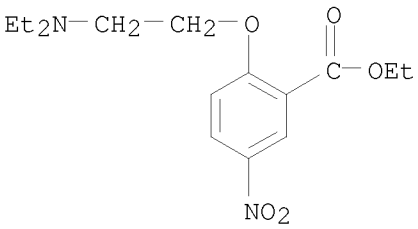
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2847344		19580812	US 1956-606795	19560829 <--

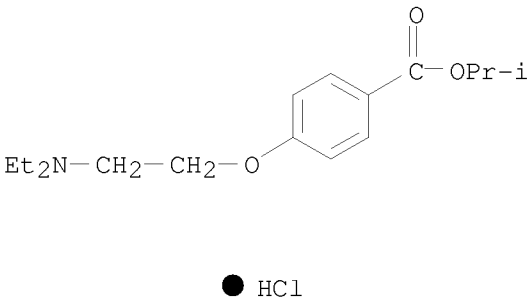
AB The title compds. (I), 5,2-Z(R2O2C)C6H3OXNRR1, are more active and less irritating than the isomeric lower-alkyl 4-amino-2-(lower-tertiary aminoalkylene lower-alkoxy)benzoates (cf. C.A. 48, 4589a). I are prepared by treating a lower-alkyl 5-nitro-2-hydroxybenzoate with a tertiary amino halide to yield I (Z = NO2), reduced to I (Z = NH2). A solution of NaOEt (prepared by adding 4.25 g. Na to 500 ml. anhydrous EtOH) is added to a stirred solution of 39 g. Et 5-nitro-2-hydroxybenzoate in 1600 ml. dry toluene, the suspension containing the precipitated yellow Na phenolate distilled to remove all EtOH, 27.5 g. Et2NCH2CH2Cl in 400 ml. dry toluene added, the mixture stirred at reflux 22 hrs., the precipitated salt filtered off, washed with dry C6H6, and the combined filtrate and washings concentrated in vacuo yielding Et 5-nitro-2-(2-diethylaminoethoxy)benzoate, golden-yellow oil; HCl salt, white needles, m. 150.1-1.3° (corrected) (absolute EtOH-hexane). Similarly prepared are I (Z = NO2) (R2, X, and NRR1 given): Et, Et, NMe2 [HCl salt (II), m. 161.4-3.4° (corrected)]; Et, Et, NBu2; hexyl, Et, NEt2; Me, Bu, NEt2; Et, Pr, 1-piperidyl, pale yellow, m. 56.7-7.7° (corrected) (EtOH) [HCl salt, m. 144.5-7.7° (corrected) (EtOH-ether)]; iso-Bu, Pr, 1-pyrrolidyl; Pr, Et, 2,5-dimethyl-1-pyrrolidyl; Et, Et, 4-morpholinyl; Et, Pr, 2-methyl-1-piperidyl [HCl salt, m. 94.4-105.4° (corrected)]; and Et, Et, 2,6-dimethyl-1-piperidyl [HCl salt, m. 187-90.2° (corrected)]. To a stirred boiling suspension of 48.1 g. powdered Fe in 400 ml. 50% aqueous EtOH is added 1 ml. concentrated HCl followed by the slow addition of 44.5 g. I (Z = NO2, R2 = Et, XNRR1 = CH2CH2NEt2), the mixture stirred and heated 20 min. after cessation of the exothermic reaction, treated with 10 g. NaHCO3 and filtered while hot, the filter-cake washed with hot EtOH and the combined filtrate and washings distilled in vacuo, the remaining mixture of H2O and oil extracted with EtOAc, the EtOAc exts. washed with H2O, dried over anhydrous MgSO4, and evaporated in vacuo yielding Et 5-amino-2-(2-diethylaminoethoxy)benzoate (III), dark amber oil. Excess HCl-Et2O is added to 6.4 g. III in 40 ml. EtOAc, the precipitated III.2-HCl washed with EtOAc by decantation and dissolved in 25 ml. absolute EtOH, 9.6 g. III in 50 ml. EtOAc added, and the mixture cooled yielding III.HCl, needles, m. 122.8-3.7° (corrected)(absolute EtOH-EtOAc). Similarly prepared are I (Z = NH2) (R2, X, and NRR1 given): Et, Et, NBu2; hexyl, Et, NEt2; Me, Bu, NEt2; Et, Pr, 1-piperidyl, amber oil [HCl salt, m. 178.1-80.1° (corrected) (absolute EtOH)]; iso-Bu, Pr, 1-pyrrolidyl; Pr, Et, 2,5-dimethyl-1-pyrrolidyl; Et, Et, 4-morpholinyl; Et, Pr, 2-methyl-1-piperidyl; and Et, Et, 2,6-dimethyl-1-piperidyl. II. (11.7 g.) in 150 ml. EtOH is treated with H (50 lb.) at room temperature in the presence of 1 g. 7% PdCl2 on C approx. 35 min., filtered, the filter pad washed with absolute EtOH, the filtrate evaporated to dryness in vacuo, the yellow oil dissolved in EtOAc, the solution evaporated to dryness, the residue dissolved in approx. 50 ml. EtOH, cooled, diluted with EtOAc and ether, mixed, and the solid crystalline material filtered off and recrystd. from 125 ml. iso-PrOH to yield Et 5-amino-2-(2-dimethylaminoethoxy)benzoate-HCl, m. 160.4-3° (corrected).

IT 1089321-54-9P
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(Lower-alkyl 5-amino-2-(tertiary aminoalkoxy)benzoates)
RN 1089321-54-9 CAPLUS
CN Benzoic acid, 2-[2-(diethylamino)ethoxy]-5-nitro-, ethyl ester, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L7 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1938:41768 CAPLUS
DOCUMENT NUMBER: 32:41768
ORIGINAL REFERENCE NO.: 32:5807a-c
TITLE: Amino ethers of phenolic benzoic esters
AUTHOR(S): Rohmann, C.; Koch, A.
SOURCE: Archiv der Pharmazie und Berichte der Deutschen Pharmazeutischen Gesellschaft (1938), 276, 154-64
CODEN: APBDAJ; ISSN: 0376-0367
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C. A. 30, 4160.7. In the present study the carboxy group of p-HOC6H4CO2H has been esterified with different alcs., while the HO group was etherified with Et2NCH2CH2OH. The alkaline ethers thus carry a tertiary N radical. This ever-present group stands in the p-position to a varying ester group. This arrangement conditions the local anesthetic action. With the aid of the organoleptic test, it was found that all the compds. prepared were more or less locally anesthetic. The change in activity, since the ether group remained constant, must therefore depend on the variation of the alkyl radical in the ester group. All the compds. were tested along with novocaine, tutocaine, cocaine and pantocaine with respect to their physicochem. properties, and the results obtained herein reported. Among the alkyl p-diethylaminoethoxybenzoate-HCl prepared were: Et, m. 154°; Pr, m. 103°; iso-Pr m. 146°; Bu m. 74°; iso-Bu m. 92°; allyl, m. 176-7°.
IT 1071582-57-4P
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(Amino ethers of phenolic benzoic esters)
RN 1071582-57-4 CAPLUS
CN Benzoic acid, 4-[2-(diethylamino)ethoxy]-, 1-methylethyl ester, hydrochloride (1:1) (CA INDEX NAME)


O
C— OPr-i
Et2N— CH2— CH2— O
HCl